

# One-dimensional Multiple Dirac delta potentials as a Finite Dimensional Eigenvalue Problem

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March 10, 2017

## Abstract

We give a brief exposition of the formulation of the bound states and scattering problems for the one-dimensional system of  $N$  attractive Dirac delta potentials, as an  $N \times N$  matrix eigenvalue problem ( $\Phi A = \omega A$ ) and discuss various physical results of the spectrum through the tools of linear algebra. In particular, we illustrate that the non-degeneracy theorem given in one dimensional bound states breaks down for the periodically distributed Dirac delta potential, where the matrix  $\Phi$  becomes a special form of the circulant matrix. We then show that the ground state is always non-degenerate and the associated wave function may be chosen to be positive by using the Perron-Frobenius theorem. We also prove that removing a single center from the system of  $N$  delta centers shift all the bound state energy levels upward as a simple consequence of the Cauchy interlacing theorem. In addition, we show from the Feynman-Hellmann theorem that there are least one, at most  $N$  bound states, and give a criterion for the existence of exactly  $N$  bound states using the Gershgorin theorem. Moreover, we give an explicit solution of the Lippmann-Schwinger equation in terms of the matrix  $\Phi$  and show that band gaps in the energy spectrum appear as the number of periodically located Dirac delta centers increases. We also discuss the so-called threshold anomaly and show the presence of scattering resonances, for which we obtain their Gamow vectors. Finally, we investigate the motion of the poles of the transmission coefficient two center problem.

## 1 Introduction

Dirac delta potentials or point interactions, or sometimes called contact potentials are one of the exactly solvable classes of idealized potentials, and used as a pedagogical tool to illustrate various physically important phenomena, where the de Broglie wavelength of the particle is much larger than the range of the interaction. They have various applications in almost all areas of physics, see [1]. For instance, mutually non-interacting electrons moving in a fixed crystal can be modeled by periodic Dirac delta potentials, known as the Kronig-Penney model [2]. The appearance of the band gaps in the spectrum of this model has been shown from the transmission coefficient in [3]. Another application is given by

the model consisting of two attractive Dirac delta potentials in one dimension. This is used as a very elementary model of a one-dimensional diatomic ion ( $H_2^+$ , for example) and has been discussed in some quantum mechanics textbooks [4] and [5] with more detail. More recently, the studies of one-dimensional several Dirac delta potentials based on transfer matrix techniques have been developed to illustrate some interesting scattering phenomenon, namely the so-called transmission resonances (the energies for which the scattering transmission coefficient is one), threshold anomalies (for the particular values of the parameters, the reflection coefficient goes to zero as the energy of the incoming particle approaches zero), Bloch states [6, 7, 8, 9, 10, 11], etc. From a pedagogical point of view, Green's function and the solution of the Lippmann-Schwinger equation for a single Dirac delta potential has been given in [12] and multiple scattering theory for double delta centers has been also studied through the Lippmann-Schwinger equation in [13]. Therefore, the interest of Dirac delta potentials and other one dimensional point potentials provides us with solvable (or quasi-solvable) models in quantum mechanics that give an insight for a better understanding of the basic features of the quantum theory. This makes them suitable for the purpose of teaching the discipline. In the recent pedagogical review [14], several interesting features of one-dimensional Dirac delta potentials has been illustrated, especially the bound state spectrum of delta potentials with some other exactly solvable potentials are discussed. In there, Multiple  $\delta$ -function potential has been studied in Fourier space and the bound state problem has been formulated in terms of a matrix eigenvalue problem and finally commented that the models can then be analyzed using matrix methods. In this paper, we will construct the matrix eigenvalue problem and study the details of the spectrum of the multiple Dirac delta potentials in detail.

Dirac delta potentials in one-dimension have been also studied from the purely mathematical point of view. One possibility for a rigorous treatment of them that corresponds to the intuitive notion of Dirac delta potentials [15] is based on the theory of self-adjoint extensions of symmetric operators. This helps us to define the formally written Hamiltonian for Dirac delta potentials as a self-adjoint extension of the free kinetic energy operator and they are extensively studied in the monographs [16, 17] (see [18, 19] for a pedagogical introduction to the self-adjoint extension theory and consult a more detailed historical development of the subject in the introduction of the monograph [16]). One dimensional point interactions of the form  $\delta$ , its first derivative  $\delta'$  or a combination thereof<sup>1</sup> may be used as a perturbation of a free kinetic term such as the Schrödinger [20, 21, 22, 23] or the Salpeter free Hamiltonian [24, 25, 26, 27] or in combination with another potentials. Examples of these potentials are the harmonic oscillator [28, 29, 30], the conic oscillator [31, 32], the infinite square well [33, 34] or even the semi-oscillator which has been used as a simple example of a potential showing resonances [35, 36]. There are other physical reasons to consider one-dimensional point potentials, e.g., the harmonic oscillators decorated with a Dirac delta potential is applied to the theory of Bose-Einstein condensates [37, 38, 39], and the Casimir effect is described by point potentials [40, 41, 42, 43, 44, 45, 46, 47, 48], and they are used in quantum dots [49, 50, 51] or even surface theory [52]. The discussions in the interpretation of one dimensional point potentials may be seen in [53]. Due to their relevance and interest, one-dimensional point potentials have been largely studied in the mathematical physics literature. An exhaustive account of all relevant works is overwhelming. In any case and along some papers cited before, we give here a selection of these relevant articles [54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70].

Point interactions have been also studied in higher dimensions. However, in this case the integrals become divergent for large values of momentum, i.e., ultraviolet divergences appear. To remedy this

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<sup>1</sup>This is only possible for a particular definition of  $\delta'$  compatible with  $\delta$ . Contrary to the situation with the perturbation  $\delta$ , there is some ambiguity in the literature on what an interaction of the type  $\delta'$  is.

problem, the idea of the renormalization that has been originally introduced in quantum field theory is employed. The renormalization of the coupling constant for this potential in three dimensions was first introduced by Thomas in the context of the nuclear physics [71]. The first rigorous treatment of the problem was given by Berezin and Faddeev in their pioneering work [72]. In the first step of the renormalization, different regularization schemes can be used either in coordinate space [73, 74, 75, 76] or in momentum space [77, 78, 79, 80, 81, 82, 83, 84]. The single Dirac delta potential in two and three dimensions has been also studied from Green's function point of view in [85]. A single Dirac delta potential in two dimensions is known as an instructive example of dimensional transmutation [77, 78], that is, the initial formal Hamiltonian does not contain an intrinsic energy scale since the coupling constant is dimensionless in natural units ( $\hbar = 2m = 1$ ). However, a new parameter is introduced through the renormalization procedure, which then fixes the energy scale of the system and this is called dimensional transmutation. This implies a violation of  $SO(2,1)$  symmetry of the scale invariant potential, so it is one of the simplest examples of anomaly or quantum mechanical symmetry breaking [79]. Furthermore, renormalization group equations and the  $\beta$  function have been discussed in [73, 84] and the model has been shown to asymptotically free in two dimensions. Apart from point interactions in flat two and three dimensions, they can also be defined on the infinite planar strips as a natural model for quantum wires containing impurities and onto torus (see [86, 87]) and on the two and three - dimensional Riemannian manifolds, where the renormalization is required, and this subject has been studied in [88, 89, 90]. One can also construct many-body models, where the particles are interacting through the two-body one-dimensional Dirac delta potentials, known as the Lieb-Liniger model [91] and they have been studied in great detail in the literature [92, 93, 94, 95] (also see the references in [16]). Many other field theoretical models in higher dimensions have been also constructed [96, 97].

In this paper, we first give a brief review of the bound state spectrum of the  $N$  Dirac delta potentials in one dimension by converting the time independent Schrödinger equation  $H\psi = E\psi$  for the bound states to the eigenvalue problem for an  $N \times N$  Hermitian matrix. This method is rather useful especially when we deal with large number of centers since the procedure that uses the matching conditions for the wave function at the location of the delta centers become cumbersome for large values of  $N$ . Once we formulate the problem as a finite dimensional eigenvalue problem, we show that there are at most  $N$  bound states for  $N$  centers, using Feynman-Hellmann theorem (see page 288 in [15]). After reviewing the basic parts of the model, we illustrate that there could be degeneracies even in the one-dimensional bound state problems. In other words, this simple one-dimensional toy problem for more than four centers allows us to give an explicit example of the breakdown of the well-known non-degeneracy theorem for one-dimensional bound state problems [98]. This shows us that we should not take the non-degeneracy theorem for granted particularly for singular interactions, where it may not be valid. This was first realized for the so-called one-dimensional Hydrogen atom [99], where the non-degeneracy theorem breaks down. This is one of the main results of this paper. In contrast to the degeneracies that appear in bound states, we show that the ground state is non-degenerate and the ground state wave function can be always chosen real-valued and strictly positive. In addition, we also show that all the bound state energies for  $N$  attractive Dirac delta potentials increase if we remove one center from the system. We also give the sufficient condition for the  $N$  Dirac delta potentials to have  $N$  bound states in a more detailed and simple way, which was originally given in [100]. This result is reduced to the standard well-known result for  $N = 2$ , see for instance [4].

In the scattering problem with the  $N$  Dirac delta potentials, we show that there is an explicit solution in closed analytical form in terms of the matrix  $\Phi$  to the Lippmann-Schwinger equation. Starting from this, we obtain all the scattering information (the reflections and transmission coefficients) about the

system. The explicit expressions of the reflections and transmission coefficients was already shown for a single center and two centers in the previous studies [12, 13]. Here, we generalize these results to  $N$  centers and illustrate several interesting features of one-dimensional scattering of this problem, e.g., threshold anomalies, or the transmission resonances, in a more accessible way from the Lippmann-Schwinger equation. Although these results have been discussed using the standard matching conditions and transfer matrix techniques [7, 9, 10, 11], we here show that the Lippmann-Schwinger approach to the scattering problem for  $N$  centers is even more powerful in obtaining essential features of the physics of the problem. We also discuss the resonances and the Gamow vectors associated with the decaying states for completeness. Finally, we investigate the motion of the poles of transmission coefficient for two centers and show that a bound state turns into a virtual state if the distance between the centers is less than some critical value. This phenomenon was originally shown for the rectangular well and barriers in [102, 103].

Although some of the results presented here are physically expected, it is not easy to show them from the standard way in dealing with Dirac delta potentials [15], where one needs tedious calculations and make some numerical computations when the number of centers are large. Here we formulate the bound state and scattering problem of the model in a simple way. We convert the original problem, the Schrödinger equation with multiple Dirac delta potentials, into a simple eigenvalue problem of a Hermitian finite dimensional matrix. Hence, all these results mentioned above become more transparent using some basic theorems from linear algebra, namely Perron-Frobenius theorem, the Cauchy interlacing theorem, and the Gershgorin theorem [101]. The simple proof of these theorems are given in Appendices so as not to interrupt the flow of the presentation. Our presentation is kept simple so that it is also accessible for physics students.

## 2 Bound States for $N$ Dirac Delta Potentials

We consider a particle moving in one dimension and interacting with the attractive  $N$  Dirac delta potentials located at  $a_i$  with strengths  $\lambda_i > 0$ , where  $i = 1, 2, \dots, N$ . The time independent Schrödinger equation is then given by

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \sum_{i=1}^N \lambda_i \delta(x - a_i) \psi(x) = E \psi(x) . \quad (1)$$

The above equation is actually a formal expression and its exact meaning can only be given by self-adjoint extension theory [16, 18, 19]. Here we follow a more traditional and heuristic approach used in the most quantum mechanics textbooks since the results that we obtain is completely consistent with the rigorous approach. As is well-known, the above equation can also be written as

$$H\psi = E\psi \quad (2)$$

in the operator form, where  $H = \frac{P^2}{2m} + V$  and the potential energy operator  $V$  for the above particular case in the bra-ket formalism is

$$V = - \sum_{i=1}^N \lambda_i |a_i\rangle \langle a_i| . \quad (3)$$

Here  $|a_i\rangle$  is the position eigenket. In the coordinate representation, the action of  $V$  on the state vector  $|\psi\rangle$  is

$$(V\psi)(x) = \langle x|V|\psi\rangle = \sum_{i=1}^N \lambda_i \delta(x - a_i) \psi(a_i) = \sum_{i=1}^N \lambda_i \delta(x - a_i) \psi(x) , \quad (4)$$

where we have used the fact  $\delta(x - a_i) \psi(a_i) = \delta(x - a_i) \psi(x)$ . This justifies the above formal potential operator (3) corresponds to the Schrödinger equation (1) with multiple Dirac delta potentials. Let us absorb the strengths  $\lambda_i$ 's into the bras and kets, i.e.,  $\sqrt{\lambda_i} |a_i\rangle = |f_i\rangle$  and similarly for bras. In terms of the rescaled bras and kets, the potential operator becomes  $V = \sum_{i=1}^N |f_i\rangle \langle f_i|$ . Substituting this into (2) in the coordinate representation, we obtain

$$\langle x|\frac{P^2}{2m}|\psi\rangle - \sum_{i=1}^N \langle x|f_i\rangle \langle f_i|\psi\rangle = E \langle x|\psi\rangle , \quad (5)$$

The rescaling is introduced to formulate the bound state problem in terms of an eigenvalue problem of a symmetric matrix, as we will see. Inserting the completeness relation  $\int \frac{dp}{2\pi\hbar} |p\rangle \langle p| = 1$  in front of  $|\psi\rangle$  and  $|f_i\rangle$ , we obtain the following integral equation, which is actually the Fourier transformation:

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}px} \tilde{\psi}(p) \left( \frac{p^2}{2m} - E \right) = \sum_{i=1}^N \sqrt{\lambda_i} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}p(x-a_i)} \phi(a_i) \quad (6)$$

where  $\langle x|p\rangle = e^{\frac{i}{\hbar}px}$ ,  $\langle p|\psi\rangle = \tilde{\psi}(p)$ , and  $\phi(a_i) = \langle f_i|\psi\rangle = \sqrt{\lambda_i} \psi(a_i)$ . Since two functions with the same Fourier transforms are equal, equation (6) implies that:

$$\tilde{\psi}(p) = \sum_{i=1}^N \sqrt{\lambda_i} \frac{e^{-\frac{i}{\hbar}pa_i}}{\frac{p^2}{2m} - E} \phi(a_i) . \quad (7)$$

It is interesting to remark that this solution depends on the unknown coordinate wave function at  $a_i$  and the energy  $E$ . If we use the relation between the coordinate and momentum space wave function through the Fourier transformation

$$\psi(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}px} \tilde{\psi}(p) , \quad (8)$$

and insert (7) into above for  $x = a_i$ , we obtain the following consistency relation

$$\psi(a_i) = \sum_{j=1}^N \sqrt{\lambda_j} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{e^{\frac{i}{\hbar}p(a_i-a_j)}}{\frac{p^2}{2m} - E} \phi(a_j) . \quad (9)$$

Multiplying both sides of (9) by  $\sqrt{\lambda_i}$  and separating the  $j = i$  th term, we have

$$\left[ 1 - \lambda_i \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{1}{\frac{p^2}{2m} - E} \right] \phi(a_i) - \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \sum_{\substack{j=1 \\ j \neq i}}^N \sqrt{\lambda_i \lambda_j} \left[ \frac{e^{\frac{i}{\hbar}p(a_i-a_j)}}{\frac{p^2}{2m} - E} \right] \phi(a_j) = 0 . \quad (10)$$

This equation can be written as a homogeneous system of linear equations in a matrix form:

$$\sum_{j=1}^N \Phi_{ij}(E) \phi(a_j) = 0, \quad (11)$$

where

$$\Phi_{ij}(E) = \begin{cases} 1 - \lambda_i \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{1}{\frac{p^2}{2m} - E} & \text{if } i = j, \\ -\sqrt{\lambda_i \lambda_j} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{e^{\frac{i}{\hbar} p(a_i - a_j)}}{\frac{p^2}{2m} - E} & \text{if } i \neq j. \end{cases} \quad (12)$$

As usual, the matrix elements are denoted by  $\Phi_{ij}(E)$  and the matrix itself by  $\Phi$ , so that  $\Phi = \{\Phi_{ij}(E)\}$ . Since the bound state energies must be negative, i.e.,  $E = -|E|$ , there is no real pole in the denominators of the integrands. Let us consider the integral in the off-diagonal part. The function under the integral sign has simple poles located at the points  $(p = \pm i\sqrt{2m|E|})$  in the complex  $p$ -plane. In order to calculate this integral by the residue method, we have to take into account separately the situations  $a_i < a_j$  and  $a_i > a_j$ . We show the contours for both cases in Figure 1.

We note that only the pole with sign plus (minus) lies inside the contour of integration for  $a_i > a_j$  ( $a_j > a_i$ ). Due to the exponential function, the integral over the semicircle vanishes as its radius goes to infinite [104]. Then, the value of the integral is obtained multiplying by  $2\pi i$  the residue at that point:

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{e^{\frac{i}{\hbar} p(a_i - a_j)}}{\frac{p^2}{2m} - E} = \begin{cases} \frac{m}{\hbar\sqrt{2m|E|}} \exp\left(-\sqrt{2m|E|}(a_i - a_j)/\hbar\right), & \text{if } a_i > a_j, \\ \frac{m}{\hbar\sqrt{2m|E|}} \exp\left(-\sqrt{2m|E|}(a_j - a_i)/\hbar\right), & \text{if } a_i < a_j. \end{cases} \quad (13)$$

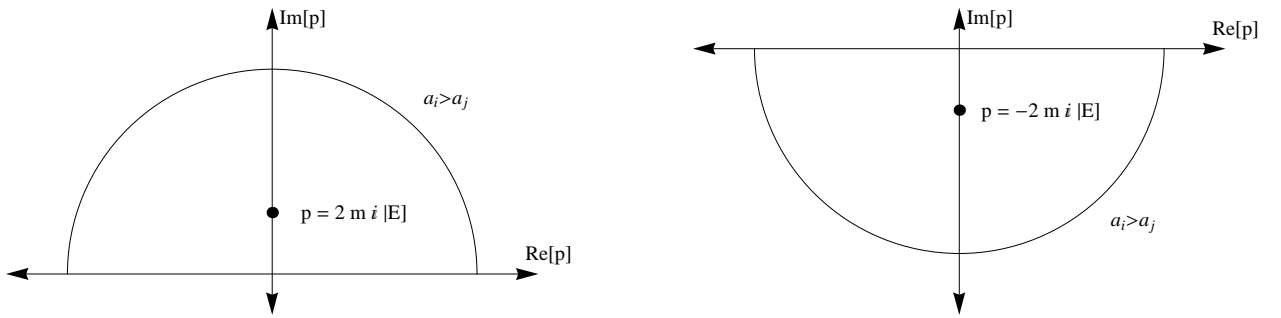


Figure 1: The contour of integration in the non-diagonal terms of the principle matrix given in Eq. (12)

The diagonal part of the matrix  $\Phi$  can be evaluated similarly, so equation (12) becomes:

$$\Phi_{ij}(E) = \begin{cases} 1 - \frac{m\lambda_i}{\hbar\sqrt{2m|E|}} & \text{if } i = j, \\ -\frac{m\sqrt{\lambda_i\lambda_j}}{\hbar\sqrt{2m|E|}} \exp\left(-\sqrt{2m|E|}|a_i - a_j|/\hbar\right) & \text{if } i \neq j. \end{cases} \quad (14)$$

Equation (11) has only non-trivial solutions if  $\det \Phi(E) = 0$ . Therefore, the bound state problem is solved once we find the solution to the transcendental equation  $\det \Phi(E) = 0$ . After that, we can find the bound state wave functions in the coordinate representation through (8). Suppose that the bound state energy, say  $E_B$ , is the root of  $\det \Phi(E) = 0$ , and we find  $\phi_B(a_j) = \sqrt{\lambda_j}\psi_B(a_j)$  from Eq.(11) associated with  $E_B$ . Then, the bound state wave function at  $a_i$  is

$$\psi_B(a_i) = \frac{1}{\sqrt{\lambda_i}} \phi_B(a_i). \quad (15)$$

Taking into account the above considerations, we use (15) into the bound state wave function in momentum space (7) so as to obtain

$$\tilde{\psi}_B(p) = \sum_{i=1}^N \sqrt{\lambda_i} \frac{e^{-\frac{i}{\hbar}pa_i}}{\frac{p^2}{2m} - E_B} \phi_B(a_i). \quad (16)$$

Then, the bound state wave function in the coordinate space can be found by just taking the inverse Fourier transform of the momentum space wave function (16).

## 2.1 Bound State Analysis for $N = 1$ and $N = 2$

For a single center located at  $x = a$  with coupling constant  $\lambda$ , the matrix  $\Phi$  is just a  $1 \times 1$  matrix, i.e., a single function:  $\Phi(E) = 1 - \frac{m\lambda}{\hbar\sqrt{2m|E|}}$ . Now, the condition  $\det \Phi(E) = 0$  means that  $\Phi(E) = 0$ , so that the bound state energy is  $E_B = -\frac{m\lambda^2}{2\hbar^2}$  for a single center [15]. After having found the bound state energy, we can find the bound state wave function. For  $N = 1$ ,  $\phi_B(a_i)$  is some constant, say  $C$ . Then, the bound state wave function in momentum space becomes

$$\tilde{\psi}_B(p) = \sqrt{\lambda} \frac{1}{\frac{p^2}{2m} - E_B} C. \quad (17)$$

The constant  $C$  can be determined from the normalization constant:

$$\lambda |C|^2 (2m)^2 \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{1}{(p^2 + \frac{m^2\lambda^2}{\hbar^2})^2} = 1. \quad (18)$$

The integral in Eq. (18) can also be evaluated using the residue theorem. However, in this case the residues are at  $p = \pm i\frac{m\lambda}{\hbar}$  and of order two. Taking the integral, we find  $C = \frac{\sqrt{m\lambda}}{\hbar}$ . Now we can find the



wave function associated with this bound state in the coordinate space by taking its Fourier transform. We perform the integration exactly as we did in (13), and obtain [15]

$$\psi_B(x) = \frac{\sqrt{m\lambda}}{\hbar} e^{-\frac{m\lambda}{\hbar^2}|x|} . \quad (19)$$

Let us first consider the special case of two centers, namely twin attractive ( $\lambda_1 = \lambda_2 = \lambda$ ) Dirac  $\delta$  potentials located at  $a_1 = 0$  and  $a_2 = a$ . Then, the expression  $\det \Phi(E) = 0$  yields to the following transcendental equation:

$$e^{-\frac{a\sqrt{2m|E|}}{\hbar}} = \pm \left( \frac{\hbar\sqrt{2m|E|}}{m\lambda} - 1 \right) . \quad (20)$$

For convenience, we define  $\kappa \equiv \frac{\sqrt{2m|E|}}{\hbar}$ . Suppose that  $\kappa_+$  ( $\kappa_-$ ) corresponds to the solution of Eq. (20) with the positive (negative) sign in front of the parenthesis, i.e.,

$$e^{-a\kappa_+} = \frac{\hbar^2\kappa_+}{m\lambda} - 1 , \quad (21)$$

or

$$e^{-a\kappa_-} = 1 - \frac{\hbar^2\kappa_-}{m\lambda} . \quad (22)$$

The bound state energies correspond to non-zero solutions for  $\kappa_{\pm}$  of the above equations (21) and (22). The first transcendental equation (21) always has one real root, which implies the presence of at least one bound state. This is clear from the following considerations: the left hand side of (21) is a monotonically decreasing function, which goes to zero asymptotically, while the right hand side is a monotonically increasing function without any asymptote. However, the second transcendental equation (22) may or may not have a real positive solution, as can be seen from the Figure 2. One real root of Eq. (22) is expected for  $\kappa_- = 0$ . However, this cannot correspond to a bound state. In order to obtain a non trivial root, we must impose the condition that the slope of the right hand side of (22) must be smaller than the slope of the left hand side in absolute value as can be seen from Figure 2, i.e.,

$$\left| \frac{d}{d\kappa} \left( 1 - \frac{\hbar^2\kappa}{m\lambda} \right) \right|_{\kappa=0} < \left| \frac{d}{d\kappa} (e^{-\kappa a}) \right|_{\kappa=0} . \quad (23)$$

This means that the distance between the centers must be greater than some critical value for two bound states:

$$a > \frac{\hbar^2}{m\lambda} . \quad (24)$$

The condition (24) corresponds to the case  $\lambda = 2$  in Fig. 23. Hence, we conclude that there are at most two bound states for attractive twin Dirac delta potentials. The first one appears unconditionally so that it corresponds to the ground state. On the other hand, the second bound state appears only if  $a$  is sufficiently large ( $\frac{\hbar^2}{ma\lambda} < 1$ ). This corresponds to the excited state of the system.

Actually, the solutions of the transcendental equations (21) and (22) can also be explicitly expressed in terms of Lambert  $W$  function. The Lambert function  $y = W(x)$  is given [105] by the solution of the transcendental equation

$$y e^y = x . \quad (25)$$



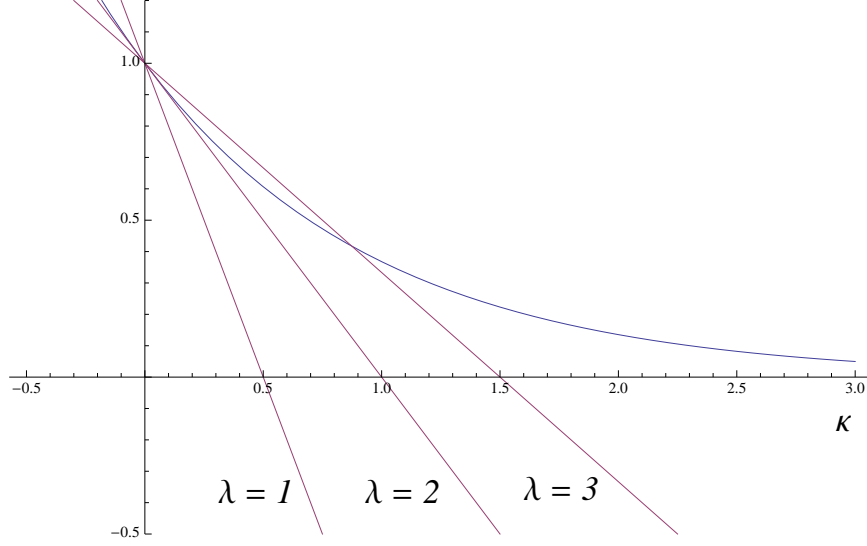


Figure 2: Right hand and left hand side of Eq. (22) as a function of  $\kappa_-$ . We take  $\hbar = 1$ ,  $m = 1/2$  and  $a = 1$  in this figure.

This function emerges in several areas in physics as well [105]. Thus, the solution to Eq. (21) and (22) turns out to be

$$E_{\pm} = -\frac{\hbar^2}{2m} \left[ \frac{m\lambda}{\hbar^2} + \frac{1}{2a} W \left( \pm \frac{ma\lambda}{\hbar^2} \exp \left( -\frac{ma\lambda}{\hbar^2} \right) \right) \right]^2. \quad (26)$$

Thanks to the Lagrange inversion theorem, we have a Taylor expansion of the Lambert  $W$  function at  $x = 0$ . This theorem states that if  $f$  is an analytic function of the variable  $y$  of the form  $f(y) = x$  at one point, then there is an explicit formula for the Taylor expansion of  $y$  at this point [105]. Then,

$$W(x) = \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{n!} x^n. \quad (27)$$

This expansion implies that

$$E_{\pm} \rightarrow -\frac{m\lambda^2}{2\hbar^2}, \quad \text{as } a \rightarrow \infty. \quad (28)$$

Hence, the eigenvalues become degenerate when the centers are infinitely far away from each other and equal to the result for the bound state energy of a single center case. This is what one intuitively may expect, since the particle interacts with one center only, while the other one is infinitely far away.

## 2.2 Bound States as a Finite Dimensional Eigenvalue Problem

In order to study location and properties of bound states more systematically, we consider the equation (11) as the particular case of an eigenvalue problem for the matrix  $\Phi$ :

$$\Phi(E) A(E) = \omega(E) A(E), \quad (29)$$

where  $\omega$  is any of the eigenvalues of the matrix  $\Phi$ . Then, the zeros of the eigenvalues of  $\Phi$  are just the bound state energies. In other words, the roots of the equation

$$\omega(E) = 0 \quad (30)$$

give the bound state energies. Hence, the eigenvalues of the *linear* differential equation  $H\psi(x) = E\psi(x)$  are obtained through a *non-linear* transcendental algebraic problem,  $\omega(E) = 0$ .

Let us go back to  $N = 2$  case. For twin centers, located at  $a_1 = 0, a_2 = a$ , the eigenvalues can be explicitly calculated:

$$\begin{aligned} \omega_1 &= 1 + \frac{m\lambda}{\hbar\sqrt{2m|E|}} \left( -1 - e^{-\frac{1}{\hbar}\sqrt{2m|E|}a} \right) \\ \omega_2 &= 1 + \frac{m\lambda}{\hbar\sqrt{2m|E|}} \left( -1 + e^{-\frac{1}{\hbar}\sqrt{2m|E|}a} \right) \end{aligned} \quad (31)$$

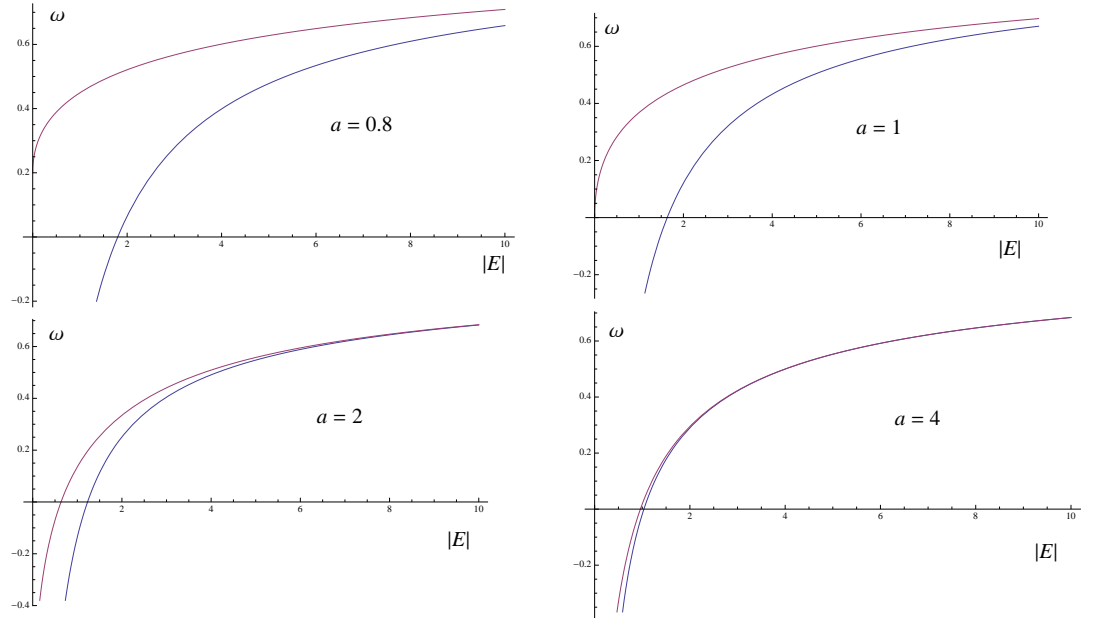


Figure 3: The flow of the eigenvalues of the matrix  $\Phi$  as a function of  $|E|$  for different values of  $a$ . Here  $\lambda = 2$  and  $\hbar = 2m = 1$ .

As shown in above Fig. 3, there are always two eigenvalues of the matrix  $\Phi$ . However, for  $\lambda = 2$  with  $\hbar = 2m = 1$ , there are two bound states only if the distance between the centers is greater than the critical value  $a = 1$ . Otherwise there is only one bound state, that is consistent with what we have discussed previously. When the centers are sufficiently close to each other, one of the bound states seems to disappear, since the zeros of the first eigenvalue seems to move to the negative real axis. We shall come back to this issue later in our discussion on the virtual states.

We also observe from Fig. 3 that the bound state energies come closer and closer as the distance between them increases. This is not surprising since the eigenvalues (31) converge to  $1 - \frac{m\lambda}{\hbar\sqrt{2m|E|}}$  as

$a \rightarrow \infty$  so that zeroes of these degenerate eigenvalues lead to degenerate bound states in the limiting case.

Now, we shall show why our method is much easier to investigate the bound state spectrum as we increase the number of Dirac delta potentials. The number of bound states is an important characteristic of any system. There are several ways to determine it for some regular potentials [106]. It is noteworthy that we can determine the maximum number of bound states of this system from the behavior of the eigenvalues of the matrix  $\Phi(E)$  through the Feynman-Hellmann theorem [107, 108].

To find the behavior of the eigenvalues as a function of  $E$ , let us first take the derivative of  $\Phi_{ij}(E)$  with respect to  $E$ . We may interchange this derivative and the integral sign in (14), since all the matrix elements  $\Phi_{ij}$  are analytic functions on the half plane  $\Re(E) < 0$ . Hence, we obtain

$$\frac{d\Phi_{ij}}{dE} = -\sqrt{\lambda_i \lambda_j} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{e^{\frac{i}{\hbar}p(a_i - a_j)}}{(\frac{p^2}{2m} - E)^2}. \quad (32)$$

Now, let us make use of the Feynman-Hellmann theorem, which states that

$$\frac{d\omega(E)}{dE} = \langle A^k | \frac{d\Phi_{ij}}{dE} | A^k \rangle, \quad (33)$$

where  $A^k$  is a given normalized eigenvector for  $\omega(E)$ . In other words, the Feynman-Hellmann theorem states that the derivative of the eigenvalue of a parameter dependent Hermitian matrix is equal to the expectation value of the derivative of the matrix with respect to its normalized eigenvector. The Feynman-Hellmann theorem can be generalized for the degenerate states [109] but it does not change our conclusion that we will draw. Thus, we have

$$\begin{aligned} \frac{d\omega(E)}{dE} &= -\sqrt{\lambda_i \lambda_j} \sum_{i,j=1}^N (A_i^k)^* \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{e^{\frac{i}{\hbar}p(a_i - a_j)}}{(\frac{p^2}{2m} - E)^2} A_j^k \\ &= -\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{1}{(\frac{p^2}{2m} - E)^2} \left| \sum_{i=1}^N e^{-\frac{i}{\hbar}pa_i} \sqrt{\lambda_i} A_i^k \right|^2 < 0. \end{aligned} \quad (34)$$

For  $E = -|E|$ ,  $\frac{d\omega(E)}{d|E|} > 0$ . Since there are at most  $N$  distinct eigenvalues of the  $N \times N$  matrix  $\Phi$  and these eigenvalues are monotonically increasing functions of  $|E|$ , there must be at most  $N$  bound states. This conclusion would have been rather difficult to arrive just by following the standard method, in which the properties of the bound states are just determined by matching conditions at the locations of the delta centers.

### 2.3 Degeneracies in the Bound States for Periodically Distributed Centers

Let us consider  $N$  Dirac delta potentials located equidistantly, i.e.,  $a_1 = 0, a_1 = a, a_2 = 2a, \dots, a_N = Na$  and  $\lambda_1 = \dots = \lambda_N = \lambda$ . Then, the matrix  $\Phi$  given in Eq. (14) takes the following form

$$\begin{pmatrix} c_0 & c_1 & \cdots & c_{N-2} & c_{N-1} \\ c_{N-1} & c_0 & c_1 & \cdots & c_{N-2} \\ c_{N-2} & c_{N-1} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & c_1 \\ c_1 & c_2 & \cdots & c_{N-1} & c_0 \end{pmatrix}_{N \times N} \quad (35)$$

where  $c_0 = 1 - \frac{m\lambda}{\hbar\sqrt{2m|E|}}$  and

$$c_j = c_{N-j} = -\frac{m\lambda}{\hbar\sqrt{2m|E|}} \exp\left(-\sqrt{2m|E|}ja/\hbar\right) \quad (36)$$

for all  $j = 1, \dots, N-1$ . The form of the matrix above (35) is usually known as the circulant matrix. By using the Fourier matrix, it can be diagonalized and its eigenvalues can be found easily [101]. However, showing this is beyond the scope of the main aim of this paper. Nevertheless, it is a simple exercise to show that

$$\begin{pmatrix} c_0 & c_1 & \cdots & c_{N-2} & c_{N-1} \\ c_{N-1} & c_0 & c_1 & \cdots & c_{N-2} \\ c_{N-2} & c_{N-1} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & c_1 \\ c_1 & c_2 & \cdots & c_{N-1} & c_0 \end{pmatrix} \begin{pmatrix} 1 \\ \zeta^l \\ \zeta^{2l} \\ \vdots \\ \zeta^{(N-1)l} \end{pmatrix} = \lambda_l \begin{pmatrix} 1 \\ \zeta^l \\ \zeta^{2l} \\ \vdots \\ \zeta^{(N-1)l} \end{pmatrix}, \quad (37)$$

where  $\zeta$  is the  $N$ th root of the unity, i.e.,  $\zeta = e^{2\pi i/N}$  and  $j = 0, 1, \dots, N-1$  and  $\lambda_l$ 's are the eigenvalues of the matrix  $\Phi$ , given by

$$\omega_j = \sum_{k=0}^{N-1} c_k \zeta^{jk}. \quad (38)$$

Note that the above formula is reduced to (31) for  $N = 2$ . We realize that for  $N > 3$ , the eigenvalues are degenerate

$$\omega_j = \omega_{N-j} \quad (39)$$

for all  $j = 1, \dots, N-1$  since

$$\omega_j = c_0 + \sum_{k=1}^{N-1} c_k \zeta^{jk} = c_0 + \sum_{k=1}^{N-1} c_{N-k} \zeta^{jk} = c_0 + \sum_{l=1}^{N-1} c_l \zeta^{j(N-l)} = c_0 + \sum_{l=1}^{N-1} c_l \zeta^{(N-j)l} = \omega_{N-j}, \quad (40)$$

where we have used  $\zeta^N = 1$  and  $j(N-l) = (N-j)l \pmod{N}$  [110]. Note that  $\omega_0$  and  $\omega_N$  cannot be degenerate. Since the matrix  $\Phi$  is Hermitian, its algebraic multiplicity is equal to its geometric multiplicity<sup>2</sup>, the eigenvectors  $A_j$  associated with the degenerate eigenvalues  $\omega_j$  span the degenerate space. Since the functions  $\omega_j(E)$  are monotonic functions of  $|E|$ , there exists a one-to-one relation between  $\omega_j(E)$  and its zeros. From the monotonic behavior of the eigenvalues  $\omega_j(E)$  and the explicit relation between the bound state wave function and the eigenvectors  $A_j$ , we conclude that the bound state energies are degenerate and the dimension of the degeneracy subspace of  $\Phi$  is equal to the dimension of the degeneracy subspace of the bound state wave functions. This is contrary to the common belief that there is no degeneracy in one-dimensional bound state problems [98]. Actually, it has been demonstrated long time ago that there exist one-dimensional singular potentials (e.g., one dimensional Hydrogen atom), where degeneracies may occur [99]. This contradiction is actually coming from an implicit assumption in the standard proof [98]. However, this assumption breaks down for singular potentials. Therefore, we highlight the fact that we should not take the non-degeneracy theorem in one-dimensional bound state problems for granted and be aware of the fact that there are some singular potentials in one dimension that admit degeneracies.

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<sup>2</sup>The algebraic multiplicity of an eigenvalue  $\lambda$  is the number times it is repeated as a root of the characteristic polynomial, whereas the geometric multiplicity of  $\lambda$  is the maximal number of linearly independent eigenvectors associated with  $\lambda$ .

## 2.4 Non-degeneracy of the Ground State

For a generic distribution of centers, it is not obvious whether the ground state is non-degenerate or not. Here, we shall show that this is indeed the case by using the Perron-Frobenius theorem (see page 661 in [101]) for symmetric matrices. Let us first recall the Perron-Frobenius theorem:

Let  $A = (a_{ij})$  be an  $N \times N$  symmetric matrix with elements  $a_{ij} > 0$  and let  $\lambda$  be the largest eigenvalue. Then,

1.  $\lambda > 0$ .
2. There exists a corresponding eigenvector  $(x_j)$  with every component  $x_j > 0$ .
3.  $\lambda$  is non-degenerate.
4. If  $\mu$  is any other eigenvalue,  $\lambda > |\mu|$ .

In order to make our presentation self-contained, an elementary proof (just using the basic knowledge of linear algebra) of this theorem is given in Appendix A [111].

Since the matrix  $\Phi$  given in (14) is symmetric but not positive, we can not directly apply the Perron-Frobenius theorem. Nevertheless, we can make  $\Phi$  positive in such a way that the spectrum of the problem is invariant. One simple way to achieve this is to subtract from  $\Phi$  a diagonal matrix whose elements coincide with the maximum of the diagonal elements of  $\Phi$  and, then, reversing the overall sign:

$$\Phi'(E) := - \left[ \Phi(E) - (1 + \varepsilon) \max_{E_{gr} \leq E < \infty} \text{diag}(\Phi_{11}(E), \dots, \Phi_{NN}(E)) \right] > 0, \quad (41)$$

where  $\varepsilon$  is arbitrarily small positive number. Let  $E_{gr}$  be the ground state energy. Since  $\Phi_{ii}(E)$  is a decreasing function of  $E$ ,  $\max_E \Phi_{ii}(E) = \Phi_{ii}(E_{gr})$ . Let us simplify this further by replacing  $\Phi_{ii}(E_{gr})$  with  $\max_i \Phi_{ii}(E_{gr}) =: \Phi(E_{gr}, \lambda_{min})$ , where  $\lambda_{min} := \min_i \lambda_i$ . Here, we have used the fact that  $\Phi_{ii}$  is a decreasing function of  $\lambda_i$ . Then, we define

$$\Phi''(E) := - [\Phi(E) - (1 + \varepsilon) I \Phi(E_{gr}, \lambda_{min})], \quad (42)$$

where  $I$  is the identity matrix. Adding a diagonal matrix to  $\Phi$  does not change its eigenvectors whereas its eigenvalues are shifted by a constant amount. However, this is equivalent to an overall translation in the bound state spectrum, which is physically unobservable. Hence, the transformed positive matrix  $\Phi''$  and  $\Phi$  have common eigenvectors and this guarantees that there exist a strictly positive eigenvector  $A$  for  $\Phi''$  and

$$\Phi''(E)A(E) = - [\omega(E) - (1 + \varepsilon) I \Phi(E_{gr}, \lambda_{min})] A(E) = \omega''(E) A(E). \quad (43)$$

The minimum eigenvalue of  $\Phi$  corresponds to the maximum eigenvalue of  $\Phi''$ . For a given  $E$ , there exists a strictly negative non-degenerate minimum eigenvalue of  $\Phi$ , say  $\omega^{min}(E)$  as a consequence of the Perron-Frobenius theorem. Since we are looking for the zeros of the eigenvalues  $\omega(E)$ ,  $\omega^{min}$  goes to zero at the ground state energy  $E_{gr} = -|E_{gr}|$ , as can be easily seen in Fig. 4. In other words, we must have

$$\omega^{min}(E_{gr}) = 0. \quad (44)$$

Then, from the remaining part of the Perron- Frobenius theorem, we conclude that there exists a corresponding positive eigenvector  $A_i(E_{gr})$  associated with the non-degenerate minimum eigenvalue  $\omega^{min}(E_{gr})$ . Using

$$\begin{aligned}\psi_{gr}(x) &= \sum_{i=1}^N \sqrt{\lambda_i} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \left( \frac{e^{\frac{i}{\hbar}p(x-a_i)}}{\left(\frac{p^2}{2m} + |E_{gr}|\right)} \right) A_i(E_{gr}) \\ &= \sum_{i=1}^N \sqrt{\lambda_i} A_i(E_{gr}) \left( \frac{m}{\hbar\sqrt{2m|E_{gr}|}} \exp\left(-\sqrt{2m|E_{gr}|}|x - a_i|/\hbar\right) \right),\end{aligned}\quad (45)$$

we also conclude that  $\psi_{gr}(x)$  is positive so it has no node.

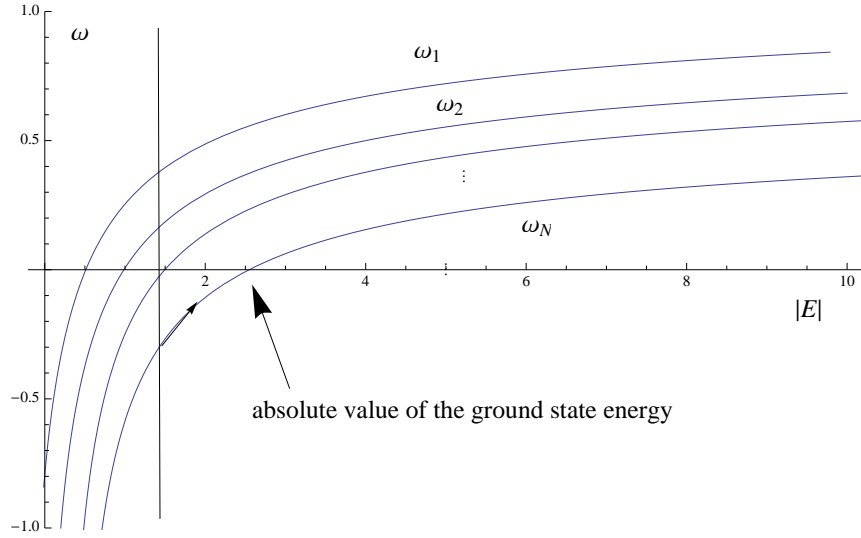


Figure 4: Flow of the eigenvalues of  $\Phi$

Another important result about the bound states is that the ground state energy increases when we remove one of the centers from the system. This can be seen from the Cauchy interlacing theorem and the monotonic behavior of the eigenvalues  $\omega$  of the matrix  $\Phi$ . The Cauchy interlacing theorem states the following (page 552 in [101]):

Let  $A$  be a Hermitian matrix of order  $N$  and let  $B$  be a principal submatrix of  $A$  of order  $N - 1$ . Let us list the eigenvalues of  $A$  in decreasing order as  $\lambda_N \leq \lambda_{N-1} \leq \dots \leq \lambda_2 \leq \lambda_1$  and the same with the eigenvalues of  $B$  as  $\mu_N \leq \mu_{N-1} \leq \dots \leq \mu_2$ . Then, we have

$$\lambda_N \leq \mu_N \leq \lambda_{N-1} \leq \mu_{N-1} \leq \dots \leq \lambda_2 \leq \mu_2 \leq \lambda_1. \quad (46)$$

A simple proof of this theorem using the intermediate value theorem in Calculus is given in Appendix B. Suppose now that we have  $N$  Dirac delta centers along with the associated  $N \times N$  matrix  $\Phi$ . As we remove one single center, its spectrum is determined from the principal submatrix of  $\Phi$  of order  $N - 1$ . From Cauchy interlacing theorem, the eigenvalues of the matrix  $\Phi$ , with order  $N$ , are interlaced with those of any principal submatrix of  $\Phi$  of order  $N - 1$ . This means that the minimum eigenvalue of the principal submatrix of  $\Phi$  is greater than or equal to the minimum eigenvalue of  $\Phi$ . Since the eigenvalues

are increasing functions of  $|E|$ , we conclude that new minimum eigenvalue goes to zero at a lower point in the  $|E|$  axis. Hence, the ground state energy increases for the new system. Actually, this argument can be applied to all other bound states as well. In other words, the bound state spectrum is shifted upwards as we remove one center from the system.

## 2.5 Sufficient Condition for the Maximum Number of Bound States

Previously, we have discussed the criteria to have exactly two bound states for twin centers. Let us look for sufficient conditions for having exactly  $N$  bound states for  $N$  arbitrarily distributed attractive Dirac delta potentials with equal strengths, i.e.,  $\lambda_1 = \lambda_2 = \dots = \lambda_N$ . This is a rather hard problem if we follow the standard approach based on the analysis of the matching conditions at the points supporting the deltas. Here we illustrate a powerful approach originally introduced in [100] (see also [112]) and it is essentially based on the Gershgorin's theorem (page 498 in [101]).

It is natural to expect that the eigenvalues  $\omega_i(E)$  of the matrix  $\Phi$  are continuously differentiable function of  $|E|$  since  $\Phi$  is a Hermitian continuously differentiable matrix for all  $|E| > 0$  (each entries of  $\Phi$  are continuously differentiable function, see Eq. (14)). This can be rigorously proved, see Theorem II.6.8 in [113]. Moreover, since  $\lim_{|E| \rightarrow \infty} \Phi_{ij}(E) = \Phi_{ii}(E) = I$ ,  $I$  being the unit matrix, we may expect that  $\lim_{|E| \rightarrow \infty} \omega_i = 1$  for all  $i = 1, 2, \dots, N$ . This implies that  $\omega_i(|E|) > 0$  for large enough  $|E|$ . Suppose that all the eigenvalues  $\omega_i$  of the matrix  $\Phi_{ij}$  are negative for some sufficiently small  $|E_*|$ , i.e.,  $\omega_i(|E_*|) < 0$  for all  $i$ . Then there exist exactly  $N$  of the  $|E_i|$  such that  $\omega_i(|E_i|) = 0$  for all  $i$  due to the intermediate value theorem [114]. Hence, it implies that  $\det \Phi(|E_i|) = 0$ , for which  $-|E_i|$  is a bound state energy. The monotonic behaviour of  $\omega_i$ 's guarantees that there exist exactly  $N$  of the  $|E_i|$ 's for which  $\omega_i(|E_i|) = 0$  for all  $i$ . Hence, if  $\Phi_{ij}(|E|)$  is negative definite, i.e., all its eigenvalues are negative, for some  $|E_*|$ , then we have  $N$  bound states.

Let us recall now Gershgorin's theorem in linear algebra [101]: All eigenvalues of a matrix  $\Phi$  are contained in the union of Gershgorin's disks

$$G_i = \left\{ z \in \mathbb{C}; |z - \Phi_{ii}| \leq \sum_{j \neq i} |\Phi_{ij}| \right\}, \quad (47)$$

for  $i = 1, \dots, N$ . We recall a simple proof of it in Appendix C.

Let

$$G_i(|E|) = \left[ \Phi_{ii}(|E|) - \sum_{j \neq i} |\Phi_{ij}(|E|)|, \Phi_{ii}(|E|) + \sum_{j \neq i} |\Phi_{ij}(|E|)| \right]. \quad (48)$$

Then, Gershgorin's theorem implies that  $\omega_i(|E|) \in \cup_{j=1}^N G_j(|E|)$  for all  $i$ . Thus, all the eigenvalues  $\omega_i(|E_*|)$  are negative and the above fact implies that if there exists  $|E_*|$  such that

$$\Phi_{ii}(|E_*|) + \sum_{j \neq i} |\Phi_{ij}(|E_*|)| < 0, \quad (49)$$

then there are  $N$  bound states. Let us now notice that

$$\max_{1 \leq i \leq N} G_i(|E|) \leq \max_{1 \leq i \leq N} \Phi_{ii}(|E|) + (N-1) \max_{1 \leq i \leq N} \max_{1 \leq j \neq i \leq N} |\Phi_{ij}(|E|)|. \quad (50)$$



For this to be negative, it is necessary that the first term  $\max_{1 \leq i \leq N} \Phi_{ii}(|E|)$  has to be negative. Let  $d = \min_{1 \leq i, j \leq N} \{|a_i - a_j|; i \neq j\}$  and  $x := \sqrt{2m|E|}$ . It is easy to see that the following condition

$$x - \frac{m\lambda}{\hbar} + (N-1) \frac{m\lambda}{\hbar} \exp\left(-\frac{d}{\hbar} x\right) < 0, \quad (51)$$

implies the condition given in (49). A sufficient condition for (51) in terms of the parameters  $\lambda$  and  $d$  requires  $x < \frac{m\lambda}{\hbar}$ .

Let  $f(x) := x - \frac{m\lambda}{\hbar} + (N-1) \frac{m\lambda}{\hbar} \exp\left(-\frac{d}{\hbar} x\right)$ . The critical point  $x_c$  on  $[0, \infty)$  can be easily found from  $f'(x) = 0$  so that  $x_c = \frac{\hbar}{d} \log\left((N-1) \frac{m\lambda d}{\hbar^2}\right)$ . Note that  $f(0) = (N-2) \frac{m\lambda}{\hbar}$ . It is easy to see that  $f$  is concave up ( $f''(x) > 0$ ) for all  $x \geq 0$ . Hence, the point  $x_c$  is a local minimum, where

$$f(x_c) = \frac{\hbar}{d} \left(1 + \log\left((N-1) \frac{m\lambda d}{\hbar^2}\right)\right) - \frac{m\lambda}{\hbar}. \quad (52)$$

Since  $\log x \leq x - 1$  for all  $x > 0$ , it guarantees that  $f(x_c) \leq f(0)$ . Then, if  $f(x_c) < 0$ , there exists at least one  $x$  such that  $f(x) < 0$  and this implies that there are  $N$  bound states. Hence, the condition  $f(x_c) < 0$  and the positivity of  $x_c$  give the following conditions

$$\begin{aligned} (N-1) &< \frac{\hbar^2}{m\lambda d} \exp\left(\frac{m\lambda d}{\hbar^2} - 1\right) \\ d &> \frac{\hbar^2}{m\lambda(N-1)}. \end{aligned} \quad (53)$$

These are the sufficient conditions in order to have  $N$  bound states. For  $N = 2$ , we recover the condition given in Eq. (24).

### 3 The Lippmann-Schwinger equation for $N$ Dirac delta potentials

The idea of using Lippmann-Schwinger equation in obtaining scattering information of the systems is not new. For instance, it was used in [13] as an attempt to construct a theory of multiple scattering from Dirac delta potentials by an iterative method. Here, we provide a detailed study of the exact solution of the Lippmann-Schwinger equation for our model, starting with the simplest cases  $N = 1$  and  $N = 2$ . Our method can easily be extended for larger values of  $N$  although the resulting equations become more complicated.

For simplicity it is often convenient to write the Lippmann-Schwinger equation in the momentum representation. It is basically a relation between momentum eigenkets  $|k^\pm\rangle$  corresponding to the total Hamiltonian, and momentum eigenkets  $|k\rangle$  for the free or unperturbed Hamiltonian  $H_0$ . It has the following form [115]:

$$|k^\pm\rangle = |k\rangle - G_0(E_k \pm i0)V|k^\pm\rangle. \quad (54)$$

Here  $V$  represents the potential, the signs  $+$  and  $-$  refer to the outgoing and incoming boundary conditions, respectively, and  $E_k = k^2/2m$ . We pick the positive sign since it corresponds to the physical scattering problem. The Green operator for  $H_0$ , defined as  $G_0(z) = (H_0 - z)^{-1}$ , is analytic on the complex variable  $z$  with discontinuities located at the values of the spectrum of  $H_0$ . The spectrum of the free

Hamiltonian is continuous and coincides with the positive semi-axis  $[0, \infty)$ . Then,  $G_0(E_k \pm i0)$  are the boundary values of  $G_0(z)$  on the positive real line as we approach from above (plus sign) or from below (minus sign). This idea is more often expressed as,  $\lim_{\epsilon \rightarrow 0^+} G_0(E_k \pm i\epsilon) = G_0(E_k \pm i0)$ . Since the Green's operator is discontinuous on the spectrum of the free Hamiltonian, i.e., on the positive semiaxis, both limits are different [115]. One of the interesting facts about our model is that the Lippmann-Schwinger equations admit exact solutions, which is not true in the general case where only approximate iterative solutions are known (Born approximation).

If we insert the potential  $V$  given in Eq. (3) into the Lippmann-Schwinger equation (54) and multiply the result by the bra  $\langle x|$  from the left, we obtain:

$$\langle x|k^\pm\rangle = \langle x|k\rangle + \sum_{j=1}^N \lambda_j \langle x|G_0(E_k \pm i0)|a_j\rangle \langle a_j|k^\pm\rangle. \quad (55)$$

Recall that  $\langle x|k\rangle$  is the free plane wave and that we are keeping only the  $+$  sign in Eq. (55). We find the following equation for the perturbed plane wave  $\psi_k^+(x) = \langle x|k^+\rangle$  as

$$\psi_k^+(x) = e^{ikx} + \sum_{j=1}^N \lambda_j G_0(x, a_j; E_k + i0) \psi_k^+(a_j), \quad (56)$$

where we have used the notation  $G_0(x, y; E_k + i0) = \langle x|G_0(E_k + i0)|y\rangle$ . This is the well known Green's function for the free Hamiltonian  $H_0$ . Similar to the scaling argument introduced for bound states, we define  $|f_i\rangle = \sqrt{\lambda_i}|a_i\rangle$  and  $\phi_k^+(a_i) = \sqrt{\lambda_i}\psi_k^+(a_i)$ .

In order to obtain the coefficients  $\psi_k^+(a_i)$ , we just replace  $x$  by  $a_i$  in Eq. (56) and isolate the  $j = i$  th term from the sum. Then, we obtain

$$\psi_k^+(a_i) = e^{ika_i} + \lambda_i G_0(a_i, a_i; E_k + i0) \psi_k^+(a_i) + \sum_{j \neq i}^N \lambda_j G_0(a_i, a_j; E_k + i0) \psi_k^+(a_j), \quad (57)$$

or, equivalently,

$$[1 - \lambda_i G_0(a_i, a_i; E_k + i0)] \phi_k^+(a_i) - \sum_{j \neq i}^N \sqrt{\lambda_i \lambda_j} G_0(a_i, a_j; E_k + i0) \phi_k^+(a_j) = \sqrt{\lambda_i} e^{ika_i}. \quad (58)$$

This relation can be written in a matrix form. Then, Eq. (58) has the form

$$\sum_{j=1}^N \Phi_{ij}(E_k + i0) \phi_k^+(a_j) = \sqrt{\lambda_i} e^{ika_i}, \quad i = 1, 2, \dots, N, \quad (59)$$

where

$$\Phi_{ij}(E_k + i0) = \begin{cases} 1 - \lambda_i G_0(a_i, a_i; E_k + i0) & \text{if } i = j, \\ -\sqrt{\lambda_i \lambda_j} G_0(a_i, a_j; E_k + i0) & \text{if } i \neq j. \end{cases} \quad (60)$$

Then, the solution  $\phi_k^+(a_j)$  can be easily found as

$$\phi_k^+(a_j) = \sum_{i=1}^N [\Phi^{-1}(E_k + i0)]_{ji} \sqrt{\lambda_i} e^{ika_i}, \quad (61)$$

where  $\Phi^{-1}$  is the inverse of the matrix  $\Phi$ . If we use the solution (61) in Eq. (56), we obtain:

$$\psi_k^+(x) = e^{ikx} + \sum_{i=1}^N \sum_{j=1}^N \sqrt{\lambda_i \lambda_j} G_0(x, a_i; E_k + i0) [\Phi^{-1}(E_k + i0)]_{ij} e^{ika_j}. \quad (62)$$

Let us evaluate now the free Green's function  $G_0(x, a_i; E_k + i0)$ . We insert a complete set of eigenkets of the momentum operator,  $I = \int |p\rangle \langle p| dp / 2\pi\hbar$ :

$$G_0(x, a_i; E_k + i0) = \langle x | G_0(E_k + i0) | a_i \rangle = \int_{-\infty}^{\infty} \langle x | G_0(E_k + i0) | p \rangle \langle p | a_i \rangle \frac{dp}{2\pi\hbar}. \quad (63)$$

Since  $|p\rangle$  are eigenkets of the momentum operator, we must have that  $H_0|p\rangle = \frac{p^2}{2m}|p\rangle$ . Then,

$$\langle x | G_0(E_k + i0) | p \rangle = \langle x | \frac{1}{H_0 - (E_k + i0)} | p \rangle = \frac{1}{\frac{p^2}{2m} - (E_k + i0)} e^{\frac{i}{\hbar} p x}. \quad (64)$$

Note that  $\langle p | a_i \rangle = \langle a_i | p \rangle^* = e^{-\frac{i}{\hbar} p a_i}$ , where the star denotes complex conjugation. If we use this and Eq. (64) in Eq. (63), we get:

$$G_0(x, a_i; E_k + i0) = \frac{m}{\pi\hbar} \int_{-\infty}^{\infty} \frac{e^{\frac{i}{\hbar} p(x-a_i)}}{p^2 - 2m(E_k + i0)} dp. \quad (65)$$

Before we proceed with the next step, let us recall that

$$G_0(x, a_i; E_k + i0) := \lim_{\epsilon \rightarrow 0^+} G_0(x, a_i; E_k + i\epsilon). \quad (66)$$

This remark is essential in order to understand the meaning of the integral in Eq. (65) and the term  $E_k + i0$  in Eqs.(64), (65), which is nothing but:

$$\int_{-\infty}^{\infty} \frac{e^{\frac{i}{\hbar} p(x-a_i)}}{p^2 - 2m(E_k + i0)} dp = \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{\frac{i}{\hbar} p(x-a_i)}}{p^2 - 2m(E_k + i\epsilon)} dp. \quad (67)$$

It is very important to realize that the limit and the integral in Eq. (67) cannot be interchanged. In fact, we have to solve the integral first and then proceed with the limit. Let us evaluate the integral in the right hand side of Eq. (67) by the residue method [104]. The integrand has poles at the points  $(E_k = \hbar^2 k^2 / 2m)$

$$p = \pm \hbar k \sqrt{1 + i \frac{2m\epsilon}{\hbar^2 k^2}} \simeq \pm \left( \hbar k + i \frac{m\epsilon}{\hbar k} \right), \quad (68)$$

where  $k > 0$ . In order to calculate the integral by the residue method, we have to take into account that either  $x < a_i$  or  $x > a_i$  and we choose the contours as shown in Fig. 5. We note that only the pole with

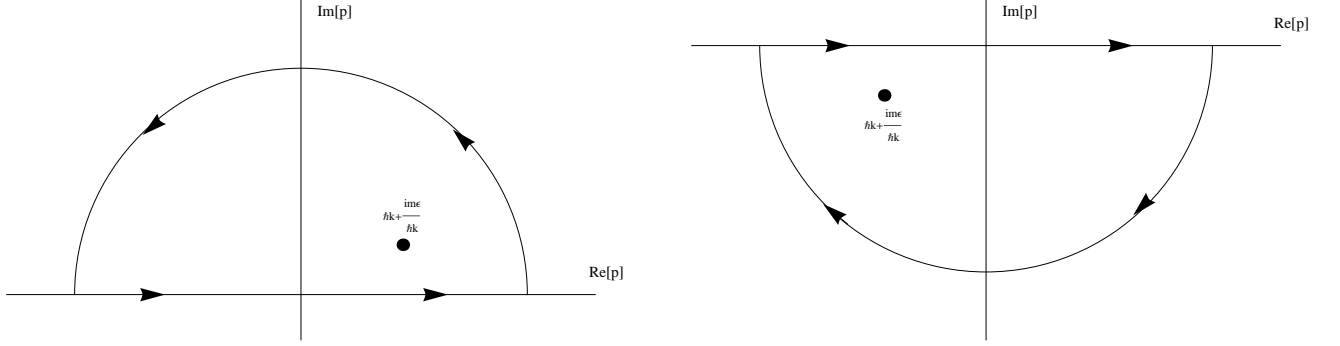


Figure 5: We choose the left contour for the residue calculation for  $x > a_i$ , and the right one for  $x < a_i$ .

plus sign in Eq. (68) lies inside the contour of integration when  $x > a_i$ . The integral over the semicircle vanishes as its radius goes to infinite. Then, from the residue theorem

$$G_0(x, a_i; E_k + i0) = \frac{im}{\hbar} \left[ \lim_{\epsilon \rightarrow 0^+} \frac{e^{\frac{i}{\hbar}(\hbar k + \frac{m\epsilon}{\hbar k})(x-a_i)}}{\hbar k + i \frac{m\epsilon}{\hbar k}} \right] = \frac{im}{\hbar^2 k} e^{ik(x-a_i)}, \quad (69)$$

for  $x > a_i$ . For  $x < a_i$  we use a similar contour defined in the lower half plane. Then, the relevant pole is the one given in Eq. (68) with the negative sign. This gives a similar result as in Eq. (69), simply replacing  $k$  in the exponential by  $-k$ . Therefore, for all values of  $x$  we can write:

$$G_0(x, a_i; E_k + i0) = \int_{-\infty}^{\infty} \frac{e^{\frac{i}{\hbar}p(x-a_i)}}{p^2 - 2m(E_k + i0)} \frac{dp}{2\pi\hbar} = \frac{im}{\hbar^2 k} e^{ik|x-a_i|}. \quad (70)$$

Substituting this result into Eq. (62), we obtain the scattering solution:

$$\psi_k^+(x) = e^{ikx} + \sum_{i=1}^N \sum_{j=1}^N \frac{im\sqrt{\lambda_i\lambda_j}}{\hbar^2 k} e^{ik|x-a_i|} [\Phi^{-1}(E_k + i0)]_{ij} e^{ika_j}, \quad (71)$$

where

$$\Phi_{ij}(E_k + i0) = \begin{cases} 1 - \frac{im\lambda_i}{\hbar^2 k} & \text{if } i = j, \\ -\sqrt{\lambda_i\lambda_j} \frac{im}{\hbar^2 k} e^{ik|x-a_i|} & \text{if } i \neq j. \end{cases} \quad (72)$$

All the information about the scattering can be obtained through this scattering solution (71) of the Lippmann-Schwinger equation.

### 3.1 The Reflection and the Transmission Coefficients

We first show that the formula (71), obtained from Lippmann-Schwinger equation, provides the results given in the standard literature [15].

For a single Dirac delta potential located at  $x = a$  with strength  $\lambda$ , formula (71) becomes

$$\psi_k^+(x) = e^{ikx} + \frac{im\lambda}{\hbar^2 k} \frac{e^{ik|x-a|}}{1 - i \frac{m\lambda}{\hbar^2 k}}, \quad (73)$$

where we have used that  $\Phi_{ii}(E_k + i0) = 1 - \frac{m\lambda_i}{\hbar\sqrt{-2m(E_k + i0)}}$  and  $\lim_{\epsilon \rightarrow 0^+} \sqrt{-2m(E_k + i\epsilon)} = -i\hbar k$ . Then, we obtain

$$\psi_k^+(x) = \begin{cases} e^{ikx} + \frac{im\lambda}{\hbar^2 k} \frac{e^{-ik(x-a)}}{1 - i \frac{m\lambda}{\hbar^2 k}} & \text{if } x < a, \\ e^{ikx} + \frac{im\lambda}{\hbar^2 k} \frac{e^{ik(x-a)}}{1 - i \frac{m\lambda}{\hbar^2 k}} & \text{if } x > a. \end{cases} \quad (74)$$

From this result, we can easily find the reflection and the transmission coefficients. Since reflection amplitude  $r(k)$  and transmission amplitude  $t(k)$  are the coefficients of  $e^{-ikx}$  and  $e^{ikx}$  in Eq. (74), respectively, we obtain the following well-known textbook result [15]:

$$R(k) = |r(k)|^2 = \frac{m^2 \lambda^2}{\hbar^4 k^2 + m^2 \lambda^2}, \quad T(k) = |t(k)|^2 = \frac{\hbar^4 k^2}{\hbar^4 k^2 + m^2 \lambda^2}. \quad (75)$$

Note that  $R + T = 1$ . Furthermore,  $T \rightarrow 1$  as  $k \rightarrow \infty$ , as expected.

If we now consider two centers located at  $a_1 = 0$  and  $a_2 = a$ , with equal strengths  $\lambda_1 = \lambda_2 = \lambda$ , the inverse of the matrix  $\Phi$  has the following form:

$$\Phi^{-1} = \frac{1}{\det \Phi} \begin{pmatrix} 1 - \frac{im\lambda}{\hbar^2 k} & \frac{im\lambda}{\hbar^2 k} e^{ika} \\ \frac{im\lambda}{\hbar^2 k} e^{ika} & 1 - \frac{im\lambda}{\hbar^2 k} \end{pmatrix}, \quad (76)$$

where

$$\det \Phi = 1 - \frac{2im\lambda}{\hbar^2 k} + \frac{m^2 \lambda^2}{\hbar^4 k^2} (e^{2ika} - 1). \quad (77)$$

These formulas are necessary in order to construct the scattering solution  $\psi_k^+(x)$  given in Eq. (71) for  $N = 2$ . The solution (62) reads for  $x < 0$ :

$$\begin{aligned} \psi_k^+(x) = e^{ikx} + \frac{im\lambda}{\hbar^2 k} e^{-ikx} \Phi_{11}^{-1} + \frac{im\lambda}{\hbar^2 k} e^{-ikx} \Phi_{12}^{-1} e^{ika} \\ + \frac{im\lambda}{\hbar^2 k} e^{-ik(x-a)} \Phi_{21}^{-1} + \frac{im\lambda}{\hbar^2 k} e^{-ik(x-a)} \Phi_{22}^{-1} e^{ika}. \end{aligned} \quad (78)$$

From (74), (76) and (77), we can obtain the reflection amplitude

$$r(k) = (\det \Phi)^{-1} \left( \frac{im\lambda}{\hbar^2 k} \right) \left[ \left( 1 - \frac{im\lambda}{\hbar^2 k} \right) (1 + e^{2ika}) + 2 \left( \frac{im\lambda}{\hbar^2 k} \right) e^{2ika} \right]. \quad (79)$$

This result is exactly the same result given in the literature obtained by imposing matching conditions of the wave function [10] for  $\lambda_1 = \lambda_2 = \lambda > 0$ .

To find the values of  $k$  for which  $T(k) = 1$ , we can use either  $r(k) = 0$  or  $R(k) = 0$ , equivalently. These are transcendental equations that must be solved numerically. Such values of  $k$  are known as *transmission resonances* in the literature. It has been shown in [10] that the energies corresponding to the transmission resonances are different from the resonance energies obtained from the poles of the  $S$  matrix or transmission coefficient. The transmission coefficient for the Dirac delta potentials located periodically in the positive real axis (the Kronig-Penney model) is depicted for different numbers of  $N$  in Fig. 6. This illustrates us the appearance of the band gaps as we increase the number of centers., which was first observed in [3].

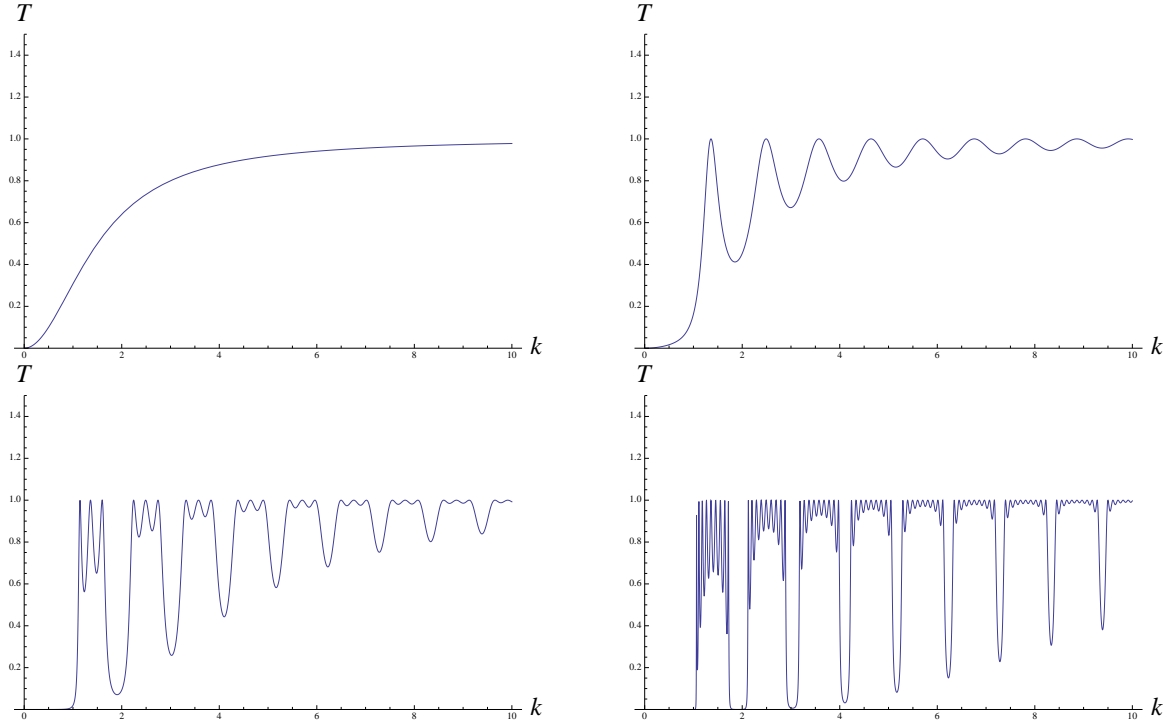


Figure 6: The transmission coefficient as a function of  $k$  for  $N = 1, 2, 4, 10$ , respectively. Here,  $\lambda_i = 2$  and  $|a_i - a_j| = 3$  for all  $i, j$ . Also we use the units such that  $\hbar = 2m = 1$ .

Now let us investigate  $R(k)$  for small values of  $k$  in more detail. To this end, let us expand it around  $k = 0$ :

$$R(k) = \left| -1 + \frac{i(-1 + \frac{2a^2m^2\lambda^2}{\hbar^4})}{2m\lambda(-1 + \frac{ma\lambda}{\hbar^2})} \hbar^2 k + O(k^2) \right|^2 \quad (80)$$

It is easy to see that  $R(k) \rightarrow 1$  as  $k \rightarrow 0$ , unless  $\frac{ma\lambda}{\hbar^2} = 1$ . This means that the reflection probability is getting closer and closer to one as the energy of the incoming particles decreases, except for the critical case  $\frac{ma\lambda}{\hbar^2} = 1$ . This is the generic case, and can be seen from Fig. 6. To understand the behavior of  $R$  near  $k = 0$  in the critical case, we first substitute  $a = \frac{\hbar^2}{m\lambda}$  into Eq.(79), and then expand near  $k = 0$  so

that

$$R(k) = \left| \frac{2ia}{3}k + \frac{16a^2}{9}k^2 + O(k^3) \right|^2. \quad (81)$$

This shows that the probability of transmission of the particle vanishes as the kinetic energy of the incoming particles are zero. This phenomenon is known as the threshold anomaly and has been first discussed in [7]. Actually, this fact can be seen more transparently by plotting the reflection coefficient as a function of  $a$  near  $k = 0$ . As can be seen from Fig. 7, the reflection coefficient sharply drops to zero

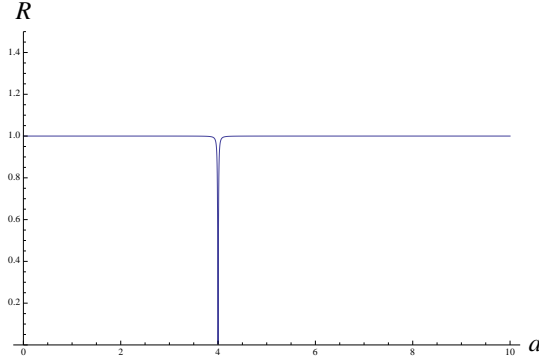


Figure 7: The reflection coefficient as a function of  $a$  for two centers. Here,  $\lambda_1 = \lambda_2 = 1/2$  and  $k = 0.01$ . Also we use the units such that  $\hbar = 2m = 1$ .

at exactly the same critical value  $a = \hbar^2/m\lambda$ . This is due to the appearance of a second bound state at this critical value. Note that this is exactly the same condition for two bound states, as discussed in the previous section. The underlying reason of this is the appearance of a bound state very close to the threshold energy [7].

### 3.2 Resonances and the Gamow states

Models with two Dirac delta potentials in the context of resonances have been discussed for instance in [116, 117] and see references therein. We recall that resonances are always produced by a perturbation on the free Hamiltonian that in our case is given by multiple Dirac delta potential  $V$ . Thus, in order to have resonances, we need a Hamiltonian pair  $(H_0, H)$ , where  $H_0$  is “free” or unperturbed and  $H = H_0 + V$ , the total Hamiltonian. We want to give here another point of view for the treatment of the model introduced in [6, 10]. In this presentation, our point of departure is the Lippmann-Schwinger equation. We shall show how to calculate the wave function and scattering coefficients for a system of  $N$  Dirac delta perturbations. Our method based on the exact solution of the Lippmann-Schwinger equations is simpler than the one given in [10]. The method in there is based on solving systems of equations using the boundary conditions for delta potentials at each delta perturbation. This becomes rather cumbersome for  $N > 2$ , whereas our method will be more efficient.

Let us emphasize a very important point about one-dimensional scattering, that has been previously mentioned. Concerning resonances and perfect transmission values, a certain confusion arises in the literature, see for example [6]. For some types of potentials there exist values of the energy for which the transmission coefficient is equal to one. They are sometimes called resonances or transmission resonances.



In [10], a terminology - *perfect transmission* - is proposed to describe this phenomenon, but we will stick to *transmission resonances*. On the other hand, we shall reserve the name of resonance for a type of the poles of the scattering  $S$  matrix. If the  $S$ -matrix is written in terms of its dependence on the momentum  $k$  of the incident particle,  $S(k)$ , and satisfies some general assumptions, then it admits an analytic continuation to the complex values of  $k$ . Then resonances are characterized by pairs of poles of  $S(k)$  located in the lower half plane symmetrically with respect to the imaginary axis. These pairs of poles reveal the existence of quantum unstable states *or* resonances, both terms denote the same physical reality. One can find a deep and thoroughly study of this in [118, 119].

Nevertheless, the poles of the transmission coefficient coincide with the poles of the scattering  $S$  matrix [?]. Due to this fact, resonance poles can be calculated by using the transcendental equation  $\det \Phi = 0$ . We may find four types of solutions:

1.- Simple poles in the positive complex semiaxis. They have the form  $i\alpha$ , with  $\alpha > 0$ . They are associated with the bound states [119].

2.- Simple poles in the negative complex semiaxis. They have the form  $-i\alpha$ , with  $\alpha > 0$ . Its physical meaning is not always clear [120, 121, 122]. They are associated with the states called *antibound* or *virtual* states [118, 119].

3.- A possible pole at the origin. This may be associated with the situation in which causality conditions as usually stated do not hold [118].

4.- Pairs of poles of the form  $\pm k_0 - ik_1$  with  $k_0, k_1 > 0$ . Each pair of poles of this kind represents a resonance [118, 119]. In principle, these poles may have any (finite) multiplicity, although for realistic models this multiplicity is one. The number of resonance pairs of poles in systems with finite range potentials (the potential is zero outside a bounded region) is infinite.

The equation  $\det \Phi = 0$ , where  $\det \Phi$  is given by (51) is identical to the formula (28) in [10] if we identify  $a$  in our equations with  $2a$  and  $\lambda = \nu_1 = \nu_2$ . Therefore, we conclude that the results in [10] for the bound states and resonances are consistent with our results. Note that in [10], the locations of the resonance poles are given in terms of the complex energies. These complex energies are calculated using the formula  $E = k^2 \hbar^2 / 2m$ , so that if  $k = \pm k_0 - ik_1$ , then  $E \pm i\Gamma/2 = (\mp k_0 - ik_1)^2$ . In terms of complex energies, the real part  $E$  is called the resonant energy and the imaginary part is related to the mean life of the resonance [119].

It is worth mentioning that equations like (54) are written in terms of Dirac kets that, like the Gamow vectors to be discussed below, do not make sense in Hilbert space, since these vectors are not normalizable in the usual square integrable sense. They acquire full meaning in suitable extensions of Hilbert spaces to more general spaces, namely the rigged Hilbert spaces [123, 124, 125, 126]. In this paper, we discuss several scattering features that our model exhibits, e.g., resonances, Gamow wave functions which are approximate wave functions for resonances with exponential decaying time behavior.

At this point, we need to remark that the transformation  $E := k^2/2m$  transforms the function  $S(k)$  into a function  $S(E)$ , which is now defined in a two-sheeted Riemann surface, where each sheet is a complex plane, see [119]. In this case, resonance poles are complex conjugate poles located on the second sheet at the points  $E \pm i\Gamma/2$ , with  $E, \Gamma > 0$ . Both complex conjugate poles represent the same resonance.

By definition a Gamow state  $\psi$  is an eigenvector (wave function) of the total Hamiltonian  $H = H_0 + V$  having the complex eigenvalue, the resonance pole  $E - i\Gamma/2$ , so that  $H\psi = (E - i\Gamma/2)\psi$ . Then, for Gamow

wave functions  $\psi$  we have

$$e^{-\frac{i}{\hbar}tH}\psi = e^{-\frac{i}{\hbar}Et}e^{-\Gamma t/2\hbar}\psi, \quad (82)$$

so that  $\psi$  decays exponentially with time. For this reason, Gamow wave functions may be looked as state wave functions for resonances.

However, we have two problems for this interpretation. The former has to do with the self-adjointness of the Hamiltonian  $H$ . A self-adjoint Hamiltonian cannot have complex eigenvalues in a Hilbert space. The only possible solution is to extend the Hilbert space to a larger space with not normalizable wave functions so that the equation  $H\psi = (E - i\Gamma/2)\psi$  as well as Eq. (80) makes sense in this larger space. This has been done with the help of the rigged Hilbert spaces, a mathematical tool that was initially used to introduce a rigorous presentation of the Dirac formalism for quantum mechanics [123, 124, 125, 126, 127]. Note that we represent the resonance by one of the resonance poles  $E - i\Gamma/2$ . The other one will play a symmetric role which will go beyond the scope of the present paper.

The second difficulty comes from the fact that it is not clear that quantum decaying systems decay exponentially for all times. In any case, experiments have shown that exponential decay is a very good approximation for decay behavior for essentially all ranges of time, with the possible exception of very short times or very large times. Thus, Gamow wave functions can be good approximations for wave functions of decaying states for the majority values of time. In our case, being given a resonance defined by a pair of poles of the  $S$  matrix, we may construct its Gamow wave function. The method is to use an analytic continuation of equation (54) and we shall use a description of it. Technicalities can be found in [128, 129]. Let  $E_R - i\Gamma/2$  be the location of a resonance pole in the energy representation. The analytic continuation of (54) at the complex value  $k_R$  so that  $z_R := E_R - i\Gamma/2 = k_R^2\hbar^2/2m$  is given by

$$|k_R^+\rangle = |k_R\rangle - G_0(z_R)V|k_R^+\rangle. \quad (83)$$

Analytic continuation means that

$$H|k_R^+\rangle = \frac{k_R^2\hbar^2}{2m}|k_R^+\rangle = z_R|k_R^+\rangle. \quad (84)$$

Thus,  $|k_R^+\rangle$  is the Gamow vector for the resonance with resonance pole  $k_R$ . This Gamow vector in the coordinate representation is  $\psi_R(x) := \langle x|k_R^+\rangle$ , so that

$$(H\psi_R)(x) = \langle x|H|k_R^+\rangle = z_R\langle x|k_R^+\rangle = z_R\psi_R(x). \quad (85)$$

If we multiply (83) from the left by  $\langle x|$ , we obtain:

$$\langle x|k_R^+\rangle = \langle x|k_R\rangle + \sum_{i=1}^N \lambda_i \langle x|G_0(z_R)|a_i\rangle \langle a_i|k_R^+\rangle. \quad (86)$$

Let us write the complex number  $k_R$  in terms of its real and imaginary parts as  $k_R = k_r - ik_I$ . Since  $\langle x|k_R\rangle = e^{ik_R x}$  by the process of analytic continuation, Eq. (86) becomes:

$$\psi_R^+(x) = e^{ik_r x} e^{k_I x} + \sum_{i=1}^N \lambda_i G_0(x, a_i; z_R) \psi_R^+(a_i). \quad (87)$$

Following the same steps introduced before, we can find  $\psi_R^+(a_i)$  and then

$$\psi_R^+(x) = e^{ik_r x} e^{k_I x} + \sum_{i=1}^N \sum_{j=1}^N \frac{im\sqrt{\lambda_i\lambda_j}}{\hbar^2(k_r + ik_I)} e^{i(k_r + ik_I)|x - a_i|} [\Phi^{-1}(z_R)]_{ij} e^{i(k_r + ik_I)a_j}. \quad (88)$$

Now, observe that the first term in the right hand side of (87) diverges exponentially as  $x \rightarrow \infty$ . In the second term, we have a sum including the Green function for the free Hamiltonian  $H_0$ , given by

$$G_0(x, a_j; z_R) = \frac{im}{\hbar} \frac{\exp\{\frac{i}{\hbar}\sqrt{2m}z_R|x - a_j|\}}{\sqrt{2m}z_R} = \frac{im}{\hbar} \frac{\exp\{\frac{i}{\hbar}\sqrt{2m}k_r|x - a_j|\} \exp\{\frac{1}{\hbar}\sqrt{2m}k_I|x - a_j|\}}{\sqrt{2m}z_R}. \quad (89)$$

Again since  $k_I$  is positive, we observe an exponential behavior for large values of  $|x|$ . The conclusion is that Gamow wave functions cannot be normalized in the sense of square integrability, but contrary to Dirac kets or plane waves which are bounded but not square integrable, they show exponential behavior at the infinity in the coordinate representation. This behavior was sometimes called the spatial or exponential catastrophe. With a proper interpretation of Gamow wave functions in terms of generalized functions in rigged Hilbert spaces, one may show that this is far from being a catastrophe [129].

### 3.3 Virtual States for $N = 2$

We briefly summarize here the results how the location of the poles of the transmission coefficient (or  $S$ -matrix) change with respect to the distance between two attractive Dirac delta potentials within our formalism. As previously emphasized, the poles of the transmission coefficients are given by the solution of the transcendental equation  $\det \Phi(k) = 0$ .

Here we choose that  $a_1 = 0$  and  $a_2 = a$ , and the units such that  $\hbar = 2m = 1$ . Then, the complex solutions of  $\det \Phi(E_k + i0) = 0$  can be found in the lower half plane of the complex  $k$  plane. In order to figure out the motion of these poles, we plot the zero level curves of  $\Re(\det \Phi(E_k + i0))$  (blue curves in Fig. 8) and  $\Im(\det \Phi(E_k + i0))$  (red curves in Fig. 8) by fixing  $\lambda$  for different values of  $a$ . The intersections of the red and blue curves on the complex  $k$  plane are the solutions of  $\det \Phi(E_k + i0) = 0$ . As stated in the previous section, the simple poles on the positive imaginary  $k$  axis correspond to the bound states, whereas the ones in the negative imaginary  $k$  axis are interpreted as so-called virtual states. As mentioned in Section 2, there are two bound states when  $a$  is sufficiently large ( $a > \hbar^2/m\lambda$  or the critical case  $a = 2$  for particular choice of the parameter  $\lambda = 2$  in the units where  $\hbar = 2m = 1$ ) and the second bound state eventually becomes a virtual state as we decrease the distance between the centers. From Fig. 8, if the distance between the centers is  $d = 2a = 1.4$ , the second bound state pole is shifted to the negative imaginary axis. Thus, it becomes a virtual state. This phenomenon also occurs for some other potentials as well, e.g., rectangular well and barrier potentials [102, 103].

## Appendix-A: A Proof of Perron-Frobenius Theorem

We give the simple proof of the Perron-Frobenius theorem for symmetric matrices given in [111]. Since the eigenvalues of  $A$  are real and the sum of the eigenvalues are equal to the trace of  $A$ , we have  $\text{Tr } A > 0$ . Then,  $\lambda > 0$ . Let  $(u_j)$  be any real normalized eigenvector associated with the eigenvalue  $\lambda$ . Then, we have

$$Au_i = \lambda u_i = \sum_j a_{ij} u_j, \quad (A-1)$$

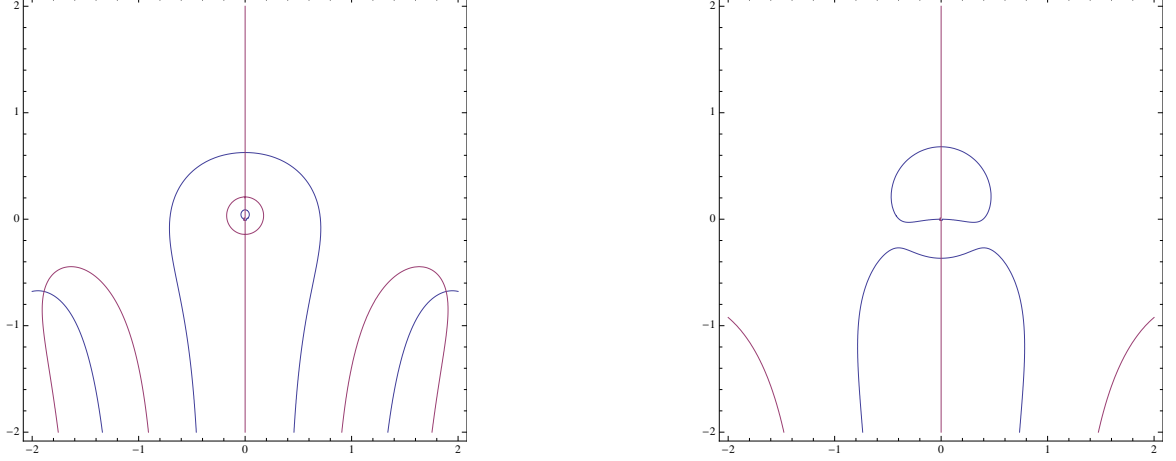


Figure 8: Contour plots of the  $\Re(\det \Phi)$  and  $\Im(\det \Phi)$  for  $a = 2.2$  on the left and  $a = 1.5$  on the right.  $\lambda_1 = \lambda_2 = 1$  in both cases.

for  $i = 1, \dots, n$ . Setting  $x_j = |u_j|$ , we get

$$0 < \lambda = \sum_{ij} a_{ij} u_i u_j = \left| \sum_{ij} a_{ij} u_i u_j \right|, \quad (\text{A-2})$$

and

$$\lambda \leq \sum_{ij} |a_{ij}| |u_i| |u_j| = \sum_{ij} a_{ij} x_i x_j. \quad (\text{A-3})$$

By means of the variational theorem, the right hand side is less than or equal to  $\lambda$  (it is equal if and only if  $(x_j)$  is the eigenvector associated with the eigenvalue  $\lambda$ ). Hence, we obtain

$$\lambda x_i = \sum_j a_{ij} x_j, \quad (\text{A-4})$$

for  $i = 1, \dots, n$ . Therefore, if  $x_i = 0$  for some  $i$ , then because of  $a_{ij} > 0$  for all  $j$ ,  $x_j = 0$  which cannot be true. Thus,  $x_j > 0$ . This completes the first two part of the theorem.

For the third part, let us assume that  $\lambda$  is degenerate. Hence, we can find two real orthonormal eigenvectors  $(u_j)$  and  $(v_j)$  associated with  $\lambda$ . Suppose that  $u_i < 0$  for some  $i$ . From the addition of Eq. (A-1) and (A-4), we have

$$\lambda(u_i + x_i) = \sum_j a_{ij} (u_j + x_j) \Rightarrow \lambda(u_i + |u_i|) = \sum_j a_{ij} (u_j + |u_j|). \quad (\text{A-5})$$

Then,  $u_j = -|u_j|$  for every  $j$ . If we assume that  $u_i > 0$  for some  $i$  and subtracting Eq. (A-4) from (A-1), we obtain  $u_j = |u_j|$ . That means  $u_j = \pm |u_j|$  and by applying the same procedure, we also have  $v_j = \pm |v_j|$ . Therefore,

$$\sum_j v_j u_j = \pm \sum_j |v_j u_j|. \quad (\text{A-6})$$

Since  $|u_j|, |v_j| \neq 0$  for all  $j$ ,  $|v_j u_j| \neq 0$  which means that  $u$  and  $v$  cannot be orthogonal. Because of the contradiction with the first assumption, we conclude that  $\lambda$  is non-degenerate.

As for the last part, let  $(w_j)$  be a normalized eigenvector associated with  $\mu$  such that  $\mu < \lambda$ ,

$$\sum_j a_{ij} w_j = \mu w_i . \quad (\text{A-7})$$

From the variational property and the non degeneracy of  $\lambda$ , we have

$$\lambda > \sum_{ij} a_{ij} |w_i| |w_j| \geq \left| \sum_{ij} a_{ij} w_i w_j \right| = |\mu| . \quad (\text{A-8})$$

## Appendix-B: A Proof of Cauchy Interlacing Theorem

Here we give a simple proof of Cauchy interlacing theorem using intermediate value theorem. This proof is originally given in [130] and we give it here in order to be self-contained. Without loss of generality, the submatrix  $B$  occupies rows  $2, 3, \dots, N$  and columns  $2, 3, \dots, N$ . Then, the matrix  $A$  has the following form:

$$A = \begin{pmatrix} a & \mathbf{y}^\dagger \\ \mathbf{y} & B \end{pmatrix} \quad (\text{B-1})$$

where  $\dagger$  denotes the Hermitian conjugation. Since  $B$  is also Hermitian, we can diagonalize it by a unitary transformation  $U$ :

$$U^\dagger B U = D , \quad (\text{B-2})$$

where  $D = \text{diag}(\mu_2, \mu_3, \dots, \mu_N)$ . For simplicity, let us define a new vector  $\mathbf{z} = (z_2, z_3, \dots, z_N)^T := U^\dagger \mathbf{y}$ , where  $T$  denotes the transposition. Here we only give the proof for the special case, where  $\mu_N < \mu_{N-1} < \dots < \mu_3 < \mu_2$  and  $z_i \neq 0$  for all  $i = 2, 3, \dots, N$ . The complete proof can be found in [130]. Let

$$V = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & U \end{pmatrix} , \quad (\text{B-3})$$

where  $\mathbf{0}$  is the zero vector. Since  $U$  is unitary,  $V$  is also unitary. It is easy to see that

$$V^\dagger A V = \begin{pmatrix} a & z^\dagger \\ z & D \end{pmatrix} . \quad (\text{B-4})$$

Let us define the following function  $f$ :

$$f(x) := \det(xI - A) , \quad (\text{B-5})$$

where  $I$  denotes the identity matrix. Since the determinant is invariant under unitary transformations, we have  $f(x) = \det(xI - V^\dagger A V)$ , or explicitly

$$f(x) = \det \begin{pmatrix} x - a & -z_2^* & -z_3^* & \cdots & -z_{N-1}^* & -z_N^* \\ -z_2 & x - \mu_2 & 0 & 0 & \cdots & 0 \\ -z_3 & 0 & x - \mu_3 & 0 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ -z_{N-1} & 0 & \cdots & 0 & x - \mu_{N-1} & 0 \\ -z_N & 0 & 0 & 0 & 0 & x - \mu_N \end{pmatrix} . \quad (\text{B-6})$$

If we expand this determinant along the first row, we get

$$f(x) = (x - a)(x - \mu_2) \cdots (x - \mu_N) - \sum_{i=2}^N f_i(x) , \quad (\text{B-7})$$

where  $f_i(x) = |z_i|^2(x - \mu_2) \cdots \widehat{(x - \mu_i)} \cdots (x - \mu_N)$  for  $i = 2, 3, \dots, N$ . Here the factor with a hat is deleted. Note that  $f_i(\mu_j) = 0$  for  $j \neq i$  and

$$f_i(\mu_i) \begin{cases} > 0 & \text{if } i \text{ is even ,} \\ < 0 & \text{if } i \text{ is odd .} \end{cases} \quad (\text{B-8})$$

Since  $f(\mu_i) = -f_i(\mu_i)$ , the sign of  $f(\mu_i)$  is opposite to that of  $f_i(\mu_i)$ . It is easy to see that  $f(x)$  is a polynomial of degree  $N$  with positive leading coefficient. Using this and the fact  $f(x)$  is the characteristic equation for the matrix  $A$ , and intermediate value theorem [114], we conclude that there exist  $N$  roots  $\lambda_1, \lambda_2, \dots, \lambda_N$  of the equation  $f(x) = 0$  such that

$$\lambda_N < \mu_N < \lambda_{N-1} < \mu_{N-1} < \cdots < \lambda_2 < \mu_2 < \lambda_1 . \quad (\text{B-9})$$

## Appendix-C: A Proof of Gershgorin Theorem

Let  $w$  be an eigenvalue of  $\Phi$ , then suppose  $\Phi \mathbf{x} = w \mathbf{x}$  where  $\mathbf{x}$  is a column vector and  $\Phi$  is a  $N \times N$  matrix. There is an element of  $\mathbf{x}$  that has largest absolute value, say  $|x_p| \geq |x_i|$  for all  $i = 1, 2, \dots, N$  and  $x_p \neq 0$ . Then,

$$wx_p = (w \mathbf{x})_p = (\Phi \mathbf{x})_p = \sum_{j=1}^N \Phi_{pj} x_j = \Phi_{pp} x_p + \sum_{\substack{i,j=1 \\ j \neq p}}^N \Phi_{pj} x_j , \quad (\text{C-1})$$

and by taking the absolute value of both sides and from the triangle inequality, we obtain

$$|w - \Phi_{pp}| |x_p| \leq \sum_{\substack{i,j=1 \\ j \neq p}}^N |\Phi_{pj}| |x_j| . \quad (\text{C-2})$$

Since  $|x_p| \geq |x_j|$ , it can be written

$$|w - \Phi_{pp}| |x_p| \leq \sum_{\substack{i,j=1 \\ j \neq p}}^N |\Phi_{pj}| |x_p| , \quad (\text{C-3})$$

and then we conclude that

$$|w - \Phi_{pp}| \leq \sum_{\substack{i,j=1 \\ j \neq p}}^N |\Phi_{pj}| . \quad (\text{C-4})$$

## Acknowledgements

The present work has been fully financed by TUBITAK from Turkey under the "2221 - Visiting Scientist Fellowship Programme". We are very grateful to TUBITAK for this support. We also acknowledge Osman Teoman Turgut for clarifying discussions and his interest in the present research. Finally, this work was also sponsored by the Spanish MINECO (MTM2014-57129-C2-1-P) and Junta de Castilla y León Project No. VA057U16.

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